Polarization of x-ray Li- and Be-like Fe satellite lines excited by an electron beam

A. S. Shlyaptseva, R. C. Mancini, and P. Neill Department of Physics, University of Nevada—Reno, Reno, Nevada 89557

P. Beiersdorfer

Lawrence Livermore National Laboratory, Livermore, California 94550

(Presented on 16 May 1996)

We have calculated the polarization properties of dielectronic satellite lines in Li- and Be-like Fe ions excited through resonance electron capture by a monoenergetic electron beam. Following the density matrix formalism, we have computed the degree of polarization and the spectral intensity distribution of dielectronic satellites associated with a given polarization state. Theoretical results were compared with experiments performed at the Livermore Electron Beam Ion Trap where satellite line emission from Fe ions was simultaneously recorded with two crystal spectrometers. These results are relevant to diagnostic applications of x-ray line polarization spectroscopy in plasmas. © 1997 American Institute of Physics. [S0034-6748(97)68401-4]

I. INTRODUCTION

Plasma diagnostic applications of x-ray line spectroscopy have proved to be very useful in helping understand plasma behavior and in the diagnosis of plasma environmental conditions for a broad range of plasma regimes. Mostly, diagnostic applications have been based on studies of atomic processes and population kinetics in plasmas which allow the calculation of line intensities, and on plasma broadening effects (e.g., Doppler, Stark, opacity) which result in characteristic lineshapes. However, the polarization properties of x-ray line emission from ions immersed in plasmas have not been extensively studied and used for diagnostic applications. For laser-produced plasmas, we are aware of only one set of measurements that shows the use of line polarization measurements on He- and Li-like Al lines for studying electron distribution functions.² The presence of fields or beams in the plasma can lead to emission of partially polarized lines from selectively populated magnetic M-sublevels. In the case of laser-produced plasmas driven by high-intensity, femtosecond-duration laser pulses, short-lived plasmas are produced whose electron distributions can show different degrees of anisotropy as well as the presence of hot electrons. The presence of beams of hot electrons in these plasmas has been inferred through the observation and analysis of K_{α} line emission in L-shell Al and Si ions induced by these energetic electrons.^{3,4} X-ray line polarization spectroscopy can lead to a more detailed characterization of hot electrons, and electron distribution functions in these plasmas.

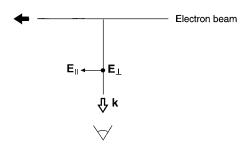
In this paper we present theoretical and experimental results for the polarization properties of K_{α} satellite line emission in Li- $(1s2l2l'-1s^22l)$ and Be-like $(1s2l2l'2l''-1s^22l2l')$ Fe ions excited by a monoenergetic electron beam through dielectronic recombination. We compare theoretical, polarization-dependent spectra with polarization-sensitive experimental spectra recorded at the Electron Beam Ion Trap (EBIT) facility of the Lawrence Livermore National Laboratory. In previous polarization studies at EBIT, the degree of polarization of $1s2l-1s^2$ transitions in He-like Sc was determined by changing the

orientation of the crystal spectrometer in separate measurements.⁵ Here, experiments were performed with Liand Be-like Fe ions and the spectra were recorded simultaneously with two crystal spectrometers: one set up to record an almost-pure polarization state parallel to the electron beam axis, and the other one set up to record a mixture of this state and the state of polarization perpendicular to the electron beam; both instruments collected radiation emitted at 90° with respect to the electron beam axis. Figure 1 displays a schematic diagram showing the directions of electron beam, observation, and states of polarization. The dispersion plane of the crystals is perpendicular to the electron beam axis. These experiments offer an excellent opportunity to benchmark theoretical results with experiments performed under well-controlled conditions before applying them to more complicated systems like laser-produced plasmas.

II. THEORETICAL POLARIZATION-DEPENDENT SPECTRA

In order to compute the satellite line intensity distributions corresponding to the different polarization states (parallel and perpendicular, Fig. 1), we calculate the total intensity of dielectronic satellite lines and multiply them by the polarization factor dependent on the polarization state and the degree of polarization of each line. All necessary atomic data were calculated with the MZ code, 6,7 namely, energies and wavelengths of the transitions, radiative transition probabilities, and autoionization rates. The MZ code is based on a perturbation theory over electrostatic interactions between electrons: the 1/Z perturbation expansion, where Z is the nuclear charge. This method was previously considered in detail for analysis of dielectronic satellite spectra produced by Fe ions in high-7 and low-density plasmas, 8 and the results of the calculations showed good agreement with the experimental data. However, this is the first time that this theory has been used to compute polarization-dependent spectra for Li- and Be-like satellite lines. We have described the polarization properties of the spectra using the photon density matrix formalism. 9,10 The degree of linear polariza-

Polarization states



Crystal selects polarization state

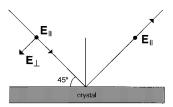


FIG. 1. Schematic diagram of the polarization states, parallel and perpendicular, relative to the direction of the electron beam, and the plane of dispersion of the crystals.

tion is expressed through nondiagonal matrix elements which depend on the population mechanism of the upper levels of the transitions. In the calculations we take into account the resonance nature of electron capture, consider that the relevant upper states in Li-like Fe (1s2l2l') are fed from the ground state of He-like Fe $(1s^2)$, and assume that the upper states in Be-like Fe (1s2l2l'2l'') are fed primarily from the ground state of Li-like Fe $(1s^22s)$. With these considerations the expression for the nondiagonal elements of the density matrix, and hence the degree of polarization, can be simplified and they depend only on the angular coupling coefficients. We have estimated that for characteristic EBIT densities ($\approx 10^{12}$ cm⁻³) the populations of first excited states $1s^22p$ are about seven orders of magnitude smaller than the population of the ground state $1s^22s$. Thus, we can reliably assume that the relevant autoionizing levels in Li- and Belike Fe are populated from the ground states of He- and Li-like Fe, respectively. Using the calculated values of the degree of polarization of dielectronic satellite lines we can calculate polarization factors for different polarization states and, hence, calculate the line intensity distribution for the parallel and perpendicular polarization states (Fig. 1). Voigt line shapes were used to describe the line intensity distribution; this includes the broadening effects associated to the radiative and autoionization decays of upper levels and the Doppler broadening due to the thermal motion of the ions in the EBIT ion trap. As an illustration of our results, Figs. 2 and 3 display theoretical spectra calculated for two values of the electron beam energy E=4620 eV and E=4695 eV, for photons emitted along a direction perpendicular to that of the electron beam axis. The electron beam energy distribution profile was assumed to be Gaussian with a FWHM=50 eV.

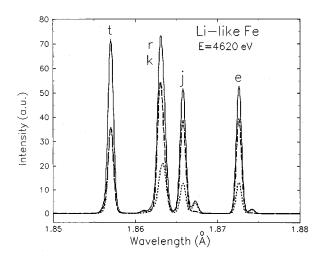


FIG. 2. Theoretical spectrum calculated for an electron beam energy E=4620 eV; (- -): intensity associated with the parallel polarization state, (···): intensity associated with the perpendicular polarization state, (—): total intensity.

For these beam energies several Li- and Be-like satellite lines are significantly excited. The spectra show the characteristic intensity distributions associated with the parallel and perpendicular polarization states (see Fig. 1) as well as the total intensity (i.e., the sum of these two). These figures clearly show lines with strong polarization like a, k, and l in Li-like Fe, lines with partial polarization like e and j in Li-like Fe and both spectral features in Be-like Fe which represent a blending of several lines, and lines with no polarization like t, m, and r in Li-like Fe (letters refer to the standard satellite line notation in Li-like ions⁶). It is also interesting to note the characteristic, relative intensity distribution associated with each polarization state. The spectra at E=4695 eV only display some of the Be-like spectral features; more Be lines become prominent for higher values of E.

III. EXPERIMENTAL DETAILS

Experiments performed at EBIT employed two von Hámos spectrometers to collect spectra simultaneously under

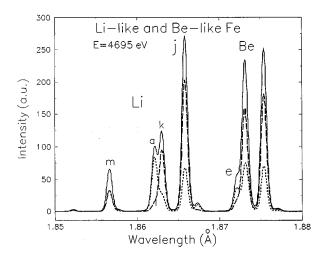


FIG. 3. Theoretical spectrum calculated for an electron beam energy E=4695 eV; (- -): intensity associated with the parallel polarization state, (···): intensity associated with the perpendicular polarization state, (—): total intensity.

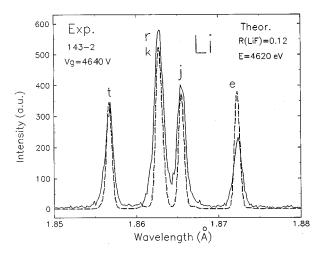


FIG. 4. Comparison of experimental spectrum recorded at V_g =4640 V (—) and theoretical spectrum calculated at E=4620 eV (- -) associated with an almost-pure, parallel polarization state.

identical experimental conditions. A schematic diagram of the Livermore EBIT and a typical high-resolution von Hámos spectrometer arrangement have been reported previously.¹¹ The spectrometers observed photons emitted in a plane perpendicular to the electron beam axis. The first used a Si(220) crystal with lattice spacing d=1.920 Å and a nominal Bragg angle of 29°. The second one used a LiF(220) crystal with d=1.424 Å and operates at a nominal Bragg angle of 41°. Each crystal was bent to a radius of curvature of $R_c = 30$ cm. The resolving power $\lambda/\Delta\lambda$ was estimated to be 1500 for the LiF, and 2200 for the Si crystal, respectively. The integrated crystal reflectivities, R_{\perp} and R_{\parallel} for x-rays polarized perpendicular and parallel, respectively, depend on the Bragg angle θ . The ratio R_{\perp}/R_{\parallel} can be expressed as $|\cos^m(2\theta)|$. The limiting values of m are m=1 for perfect crystals and m=2 for mosaic crystals. Calculations performed by Henke et al., 12 which include correction for absorption, predict values of $R_{\perp}/R_{\parallel}=0.12$ for LiF(220) and $R_{\perp}/R_{\parallel}=0.48$ for Si(220). The intensity of lines observed by the spectrometers can be expressed by $I^{\text{obs}} = R_{\parallel}I_{\parallel} + R_{\perp}I_{\perp}$,

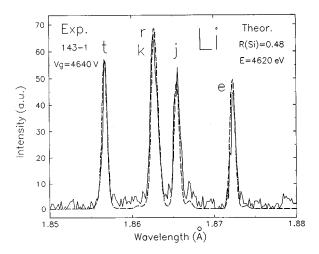


FIG. 5. Comparison of experimental spectrum recorded at V_g =4640 V (—) and theoretical spectrum calculated at E=4620 eV (- -) associated with a mixture of polarization states.

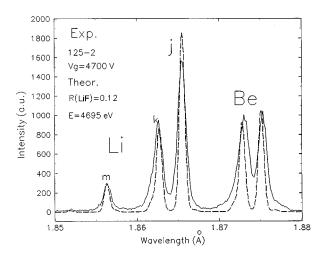


FIG. 6. Comparison of experimental spectrum recorded at V_g =4700 V (—) and theoretical spectrum calculated at E=4695 eV (- -) associated with an almost-pure, parallel polarization state.

where I_{\parallel} and I_{\perp} are the x-ray line intensity components for polarization parallel and perpendicular to the electron beam axis. Hence the observed intensity is different from the original emitted intensity due to the polarization sensitivity of the crystal. Further, the spectra recorded simultaneously by the two spectrometers will differ, due to the different reflection coefficients of the LiF(220) and Si(220) crystals. The spectrometer wavelength scales were calibrated by observing direct excitation of He-like lines $1s2l-1s^2$. Spectra were gathered at electron gun bias voltages V_g of 4600, 4640, 4700, 4750, and 4775 V. The resulting electron energy in the interaction region is subject to corrections for the middle drift tube potential and the electron beam space charge. The energy region chosen is rich with a series of dielectronic recombination resonances leading to satellite lines in Li- and Be-like Fe.

IV. DISCUSSION AND CONCLUSIONS

Figures 4–7 show the comparison between theoretical and experimental spectra collected at two different electron

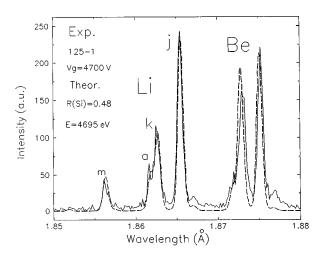


FIG. 7. Comparison of experimental spectrum recorded at V_g =4700 V (—) and theoretical spectrum calculated at E=4695 eV (- -) associated with a mixture of polarization states.

gun bias voltages V_g . Two spectra were recorded simultaneously in each experiment by two crystals: 1 (Si 220) and 2 (LiF 220). Figures 4 and 5 display experimental data at V_{g} =4640 V and theoretical results at E=4620 eV; Figs. 6 and 7 display experiment at $V_g = 4700$ V and theory at E=4695 eV. The values of electron beam energies E in the theory were selected to produce the best comparison with the experiment. Figures 4 and 6 show theory-experiment comparisons for an almost-pure parallel polarization state; the synthetic spectra were computed using the pure polarization state results displayed in Figs. 2 and 3, and the reflectivity data for the LiF crystal $(R_{\perp}/R_{\parallel}=0.12)$. Figures 5 and 7 show theory-experiment comparisons for spectra associated with a mixture of polarization states; the synthetic spectra were computed using the pure polarization state results displayed in Figs. 2 and 3, and the reflectivity data for the Si crystal $(R_{\perp}/R_{\parallel}=0.48)$. To compare with the experiment, Li spectral intensity distributions were normalized to the peaks of t(Figs. 4 and 5) and m (Figs. 6 and 7) lines; Be spectra were normalized to the peak of the longer wavelength spectral feature. The changes in the LiF- and Si-crystal experimental spectra are followed by the theory and, in general, the theory–experiment comparison is good. However, satellite e (which involves a spin-changing transition) and the blending of lines in the Be-like spectral features need more work. These preliminary results are encouraging and a more comprehensive study will be presented in a forthcoming publication.

ACKNOWLEDGMENTS

This work was supported by NSF OSR-9353227 and DOE-EPSCOR grants, and by DOE under Contract No. W-7405-ENG-48.

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